Probability Density Function Method for Variable Density Turbulence

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Variable density (VD) turbulence, as a result of the turbulent mixing of fluids with different densities, differs from incompressible shear-driven turbulence in some very fundamental ways. VD flows are present in many geophysical, astrophysical, and engineering situations. These flows are typically driven by large pressure gradients (e.g., gravity), in which the different inertias of the two different-density fluids results in large differential fluid accelerations. If the fluid configuration is unstable, i.e., the body force is directed opposite to the density gradient, small perturbations of the initial interface between the fluids grow and eventually give rise to a highly turbulent flow. This phenomenon is known as the Rayleigh-Taylor (RT) instability and its understanding and predictability are vitally important in the simulation of unstably stratified oceanic and atmospheric flows, as well as inertial confinement fusion and supernova explosions.

The computational tools used to calculate these flows are statistical turbulence closures and direct numerical simulation (DNS). DNS is an extremely useful research tool: it resolves all dynamical scales of fluid motion and provides abundant information on the flow evolution. However, its use for practical purposes is limited since it requires substantial computing power. Therefore, there is a need for statistical models that capture only certain important features of these flows, at a computational price of orders of magnitude smaller than that of DNS.

Compared with moment closures of turbulence, which traditionally solve for the first (or the first two) statistical moment of the fluctuating flow variables, probability density function (PDF) methods [1] provide a higher level statistical description by solving for the PDF, containing information on all moments. Modeling assumptions are still required, but only for two-point quantities, such as energy dissipation and molecular diffusion.

A PDF method for turbulent hydrodynamics and active scalar mixing [2,3] has been developed for VD turbulence that has the following features:

- Provides the full time-accurate evolution of the joint PDF of the fluid density and velocity in an RT-unstable flow, starting from a quiescent state and transitioning to highly nonequilibrium turbulence
- Captures the essential features of VD turbulence and mixing, such as the mixing asymmetry due to the possibly vastly different inertia of the fluids
- Correctly represents the anisotropy of the Reynolds stresses, important in predicting directional effects of turbulent mixing and the production of kinetic energy

To date statistical models cannot predict any of the above features. In addition, compared with most turbulence models developed for equilibrium flows, this method [3] surprisingly captures the time-accurate representation of the highly nonlinear process of transition to turbulence.

Compared with moment closures, PDF methods require no explicit modeling for the important physical processes of advection, chemical reactions, and the effects of mass flux: these terms appear in closed form in the sample space. The correct representation of these effects are crucial in predicting turbulent flows in general, and VD flows in particular.

In VD flows, where the densities of the mixing fluids are vastly different, the effects of large density fluctuations cannot be neglected. This is unlike the much studied and simpler class of mixing that occurs in the Boussinesq fluid case in which the densities are commensurate. In VD flows the large density differences give rise to cubic nonlinearities in the Navier-Stokes equation and mathematically very different molecular mixing rates, resulting in several non-Boussinesq effects. Examples are the mixing asymmetry, indicated by the nonzero skewness of the density PDF and the dynamic evolution of the mean pressure gradient [4]. Compared with the Boussinesq case, these features pose significant challenges for modeling. Our model is the first statistical turbulence closure to capture these recently discovered [4] VD effects.

The numerical solution of the PDF transport equation amounts to following a large number of Lagrangian particles in a Monte Carlo fashion, whose properties are governed by an equivalent system of stochastic differential equations. Thus the software implementation of the method is efficient and highly scalable.

As an example of the high-level statistical information that can be extracted from the joint PDF computed by the method, the statistical density distribution, as it evolves in time at the center of the RT mixing layer, is plotted in Fig. 1. Six different points in time are displayed for a case when the density ratio of the mixing fluids is 1:3. For validation, the density PDFs that are extracted from DNS [4] are also plotted at the same times. Figure 1 shows the excellent prediction of the full PDF at all times, representing the correct mixing state and mixing asymmetry.

The knowledge of the full PDF, provided by the method, is invaluable in the correct prediction of coupled turbulence-radiation interactions in inertial confinement fusion or astrophysical applications, combustion calculations with detailed chemistry or uncertainty quantification of hazardous releases in the atmospheric boundary layer.

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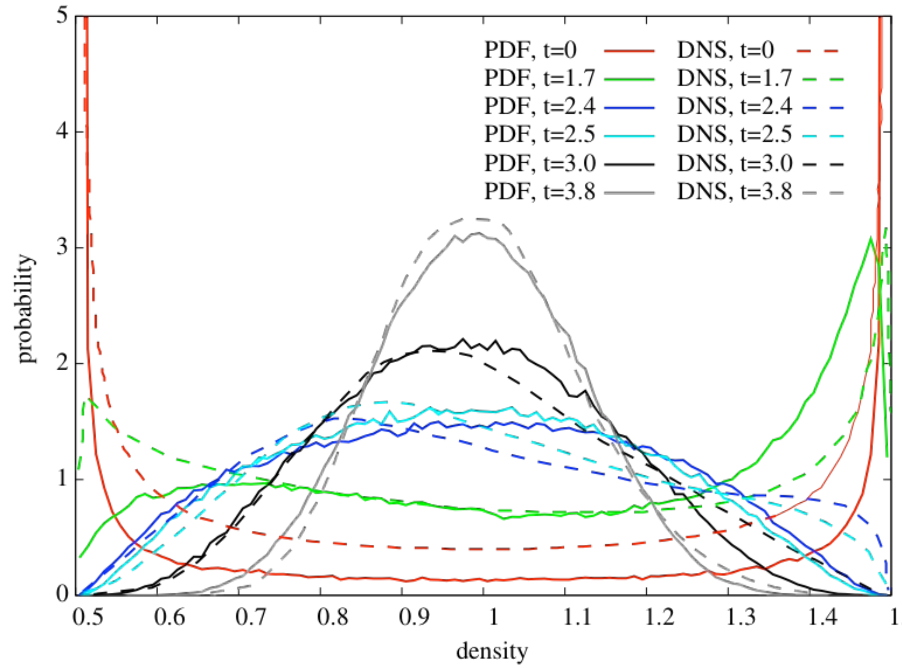

Fig. 1. Time evolution of the probability density function (PDF) of the fluid density at the center of a Rayleigh-Taylor mixing layer at the initial density ratio 1:3. Solid lines – PDF model calculation, dashed lines – direct numerical simulations (DNS) [4]. The flow starts from a quiescent state at t=0, corresponding to an approximate double-delta distribution, representing unmixed fluids. Molecular mixing, as a consequence of turbulent stirring, quickly diffuses the PDF. Variable-density (non-Boussinesq) effects already appear at this density ratio due to large differential accelerations. The higher density fluid mixes slower than the lower density one. This results in a skewed distribution, indicated by the green line at t=1.7.

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